

# A STUDY ON THE USE OF THE REACTOR BASIC EXPERIMENTS IN THE U-D<sub>2</sub>O LATTICES OF THE RB CRITICAL ASSEMBLY FOR VALIDATION OF MODERN NUCLEAR DATA LIBRARIES

by

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Demand on the availability of well-defined reactor experiments for validation of computer codes for use in nuclear industry and nuclear technology is everlasting. Users must be confident of the results obtained by the proven computer codes and nuclear data libraries chosen in the models. The well-defined (mostly historical) and evaluated reactor experiments (about 5000 in 2015) were collected continuously as the benchmarks within the frame of the OECD/NEA international projects ICSBEP (since 1995) and IRPhEP (since 2003). The Handbooks of the Projects are published in electronic forms (at the NEA web site of the OECD and at a DVD media) every year.

This study is aimed to (a) examine and evaluate reactor basic experiments, carried out in the lattice of the natural uranium metal fuel in the heavy water of the RB critical assembly first core in 1958, and (b) demonstrate their possibility for validation of modern nuclear data libraries. These RB reactor basic experiments include: (1) approach to criticality, (2) determination of the reactivity gradient at the D<sub>2</sub>O critical level, (3) measurement of the dependence of the D<sub>2</sub>O critical level on the D<sub>2</sub>O temperature, *i. e.* dependence of the reactivity with change in the D<sub>2</sub>O temperature; (4) the critical reactor geometrical parameter (buckling) measurements, (5) the migration length measurements, (6) determination of the neutron multiplication factor in the infinite lattice, and (7) the safety rods reactivity measurements. Results of the experiments are compared to the results obtained using modern nuclear data libraries of the ACE type by applying the MCNP6.1, a well-known and proven computer code based on the Monte Carlo method. A short overview of these experiments (done at the RB assembly) is shown. A brief description of the neutron ACE type nuclear data libraries (created in the LANL, based on the ENDF/B-VII.0 and ENDF/B-VII.1 files, or created in the OECD/NEA, based on the JEFF-3.2 evaluated nuclear data files), used in this validation study, is given. The benchmark models used for this validation study are described and the obtained results were analyzed. It is concluded that most of these reactor basic experiments, carried out in the lattice of the natural uranium metal fuel rods and the heavy water of the RB critical assembly, can be used as the benchmarks for validation of new nuclear data libraries. It may be done after further evaluations of influence of missing data, information and uncertainties in the material composition and geometry dimensions have been prepared according to the IRPhEP criteria and standards.

*Key words: RB reactor, U-D<sub>2</sub>O reactor experiment, MCNP6.1, nuclear data library, validation, IRPhEP*

## INTRODUCTION

The request for well-defined reactor experiments for validation of computer codes for use in nuclear industry and nuclear technologies is constant. The results obtained by the proven computer codes and nuclear data libraries have to assure the code users in their credibility. The appropriate and evaluated re-

actor experiments have been collected continuously as the benchmarks in various national and international nuclear laboratories and organizations. Nowadays, the world recognized reactor experiments benchmark systems are the OECD/NEA/NSC International Project of the Evaluated Criticality Safety Benchmark Experiments (ICSBEP [1]) and the International Reactor Physics Experiments Evaluation Project (IRPhEP [2]). These international projects contain about 5000 evaluated benchmark experiments, published in the

Handbooks, which are issued in the electronic form (as a DVD media or posted at the OECD/NEA web site) every year.

From the very beginning, with issue of the first version of the Monte Carlo based MCNP computer code (now version MCNP6.1 [3]), a great attention was dedicated to the quality assurance (QA), *i. e.* to the verification and validation (V&V) of the code, as well as to the associated nuclear data libraries. Verification of the QA includes processes that confirm that coding of the theoretical models and transport processes are errorless. Validation of the QA is a process in which the computer code results are compared to the proven and evaluated experimental systems and measured data or an analytical benchmark.

The parallel work on evaluation of nuclear data was in progress in different national nuclear data centres. The evaluated nuclear data libraries are based on (1) the proven experiments of nuclear data (shown in the internationally accepted format and collected in the Experimental Nuclear Reaction Data – EXFOR database) and (2) the well-established theoretical models implemented in various computer codes for data evaluation. These evaluated nuclear data libraries are prepared in files of the internationally accepted numerical format (now known as the ENDFB6) and disseminated in electronic form to research community since 1968. The evaluated nuclear data libraries are then processed, using various version of the NJOY [4] computer code system, to the “A Compact ENDF format”, the “continuous” (per particle energy) nuclear data libraries (known as the ACE type formatted) for use with the MCNP computer code. A recent attempt to validate different nuclear data libraries at the uranium–heavy water systems available from the evaluations published in the ICSBEP and IRPhEP Handbooks was completed in 2013 [5].

## EXPERIMENTS

A natural uranium metal fuel-heavy water critical assembly, known as the RB reactor (**R**eactor **B**), was designed in the “Boris Kidrič” (now Vinča) Institute of Nuclear Sciences, Belgrade, Serbia [6, 7]. The first criticality was achieved on April 29, 1958 [6]. The assembly aluminum cylindrical tank is mounted on an aluminum platform in a large reactor room (fig. 1). The reactor ‘bare’ core (*i. e.* without reflector) was designed without any radiation shielding and placed far away (at least 4 m) from each reflecting surface in the reactor room. In that way, neutron reflection back to the reactor tank from surrounding surfaces in the room is less than 0.4 % [6, 7]. The assembly core was constructed of 208 natural uranium metal fuel rods placed in a lattice with a square pitch of 12.0 cm in the reactor tank filled with the heavy water moderator. The reactivity of the reactor was controlled by changing the

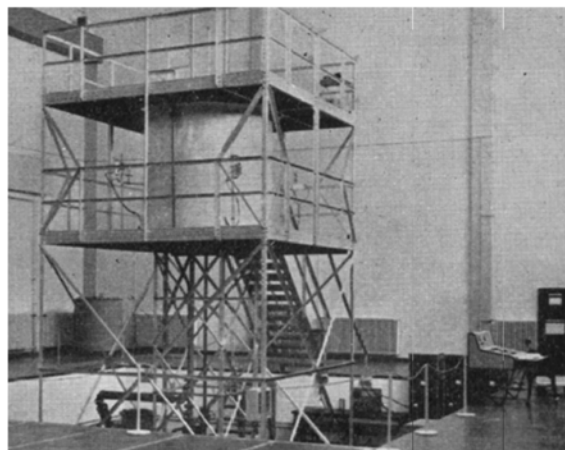


Figure 1. RB critical assembly in 1958 [6]

heavy water moderator level in the reactor tank. The RB assembly was equipped with two safety rods, installed at the reactor top cover, to shutdown reactor. The fuel forced cooling system was not provided. It is described [7] as: “The critical assembly was intended to provide: (1) experience in carrying out critical experiments, (2) operation experience with nuclear reactors, and (3) highly accurate critical conditions for heavy water – natural uranium lattices”.

The assembly was operated until October 15, 1958, when a serious reactivity-excursion accident occurred. Six operators were seriously irradiated, one with fatal outcome [8, 9]. After the *Vinča Dosimetry Experiment* [10] was carried out in April 1960, aimed to determine absorbed doses received by the staff, the assembly was modernized and modified for operation with low enriched uranium metal fuel, during the period 1960-1962.

Nevertheless, a large number of reactor basic experiments had been carried out at the RB assembly in the period from May to October 1958, before the accident occurred. These experiments included: (1) approach to criticality [6, 7], (2) determination of the reactivity gradient at the D<sub>2</sub>O critical level [11], (3) measurement of the dependence of the D<sub>2</sub>O critical level (*i. e.* the reactivity) on the D<sub>2</sub>O temperature [12]; (4) the critical reactor geometrical parameter (buckling) measurements [12], (5) the migration length measurements [11], (6) determination of the neutron multiplication factor in the infinite lattice [11], and (7) the safety rods reactivity measurements [13]. A curious question was raised recently, were these experiments, old almost 60 years, suitable for validation of data in modern nuclear libraries as possible experimental benchmarks?

From all these experiments, done in 1958, only the experiment Approach to the criticality was included (in 1999) in the ICSBEP and IRPhEP Handbooks [14]. The version 4B2 of the MCNP computer code [15] with the endf60 [16] and vmccs [17] ACE type neutron data libraries and the tmcscs [18] neutron

thermal scattering library (TSL) were used for that evaluation. Both, the code version and the neutron data libraries, are now considered obsolete. In the meantime, the most of the available (up to 2013) neutron data libraries (including TSL) of the ACE type with the (version 5.1-6) MCNP computer code [19] were used [5] in the validation process at the RB assembly first core (RB1/1958) criticality benchmark value.

Therefore, this study is aimed to evaluate all the above mentioned RB reactor basic experiments and investigate possibility for their use in validation of modern nuclear data libraries, available in the last ten years.

### Approach to the criticality

The experiment Approach to the criticality is described in [7]. The diagram of normalized inverse value of measured neutron flux density count rate in function of the D<sub>2</sub>O moderator subcritical level in the RB tank is shown in fig. 6 in [7]. The neutron flux density count rate is measured by three BF<sub>3</sub> counters placed around the tank. It was reported that the RB reactor tank was made of 99.9 % pure Al. Each natural uranium metal fuel rod had cylindrical U fuel meat with a diameter of 2.5 cm and a height of 210.0 cm. The U fuel rods were covered with 1 mm thick cladding, made of “nuclear pure” Al. The D<sub>2</sub>O moderator was reported to contain 99.82 ± 0.02 molar percent of the D<sub>2</sub>O. A Ra-Be neutron source with 17.5 GBq (0.5 Ci) Ra activity was placed in the core during subcritical measurements of the stabilized neutron flux density. The neutron source was placed in an Al guide tube along the central axis of the tank. The D<sub>2</sub>O moderator critical height was determined at the moderator level in a point in which the value of the normalized inverse flux density had approached to zero. The source and the guide tube were removed from the core at that point, and the D<sub>2</sub>O moderator critical level was determined by a fine manual adjustment of the moderator level, pumping the D<sub>2</sub>O moderator in the core and out of the core. Measured D<sub>2</sub>O moderator critical height was reported in [7] as

$$H_c = (177.60 \pm 0.10) \text{ cm, at the temperature of } 22^\circ\text{C}.$$

Measured D<sub>2</sub>O moderator critical height was also reported in [6], without any details on measurements, as

$$H_c = (177.15 \pm 0.10) \text{ cm, at the temperature of } 22^\circ\text{C}.$$

### Measurement of the reactivity gradient at the D<sub>2</sub>O critical level

The experiment Determination of the reactivity gradient at the D<sub>2</sub>O critical level is described in [11].

The experiment was conducted by measuring the stable reactor constant (*i. e.* the reactor “period”,  $T$ ) of the time dependence of neutron flux density caused by a small over-critical excess ( $\beta$ ) of the D<sub>2</sub>O moderator. The reactivity ( $\rho$ ) was determined from the measured reactor period applying the “in-hour” Nordheim formula and published data for delayed neutrons and delayed photoneutrons [11]. Not all details of the experiments were given, but from a diagram shown in fig. 2 in [11], it can be seen that about 30 different values of  $H$  were chosen up to the maximum D<sub>2</sub>O moderator excess,  $H_{\max} = 20 \text{ mm}$ .

The reactivity gradient at the D<sub>2</sub>O critical level was then determined by the least square linear fit of data shown in the  $\rho(H)$  diagram (fig. 2 in [11]) and reported as

$$\frac{d\rho}{dH}_c = 7.06 \pm 0.15 \cdot 10^{-4} \text{ cm}^{-1}$$

### Measurement of the dependence of the D<sub>2</sub>O critical level on the temperature

The experiment Measurement of the dependence of the D<sub>2</sub>O critical level on the D<sub>2</sub>O temperature is reported in [12]. Not all details of measurements were given, but from a diagram shown in fig. 1 in [12], it can be seen that the dependence of the D<sub>2</sub>O critical level ( $H_c$ ) on the D<sub>2</sub>O moderator temperature ( $T_{D_2O}$ ) was measured in the temperature range from 20 °C to 25 °C. It was claimed that no artificial heating of the moderator was used. It was assumed that the fuel and the D<sub>2</sub>O moderator in the core were at the same temperature during measurements, *i. e.* the overall (total) isothermal “temperature coefficient of reactivity” (TCR), was determined. The measured values of the  $H_c$  were in the range from 177.15 cm (at 20.5 °C) up to 178.75 (at 25 °C). Nine pairs of the measuring points  $H_c - T_{D_2O}$  were shown at the diagram  $H_c(T_{D_2O})$ . The dependence of the D<sub>2</sub>O critical level on the D<sub>2</sub>O moderator temperature was then determined by the least square linear fit of data shown in the  $H_c(T_{D_2O})$  diagram (fig. 1 in [12]) and reported (without any uncertainty) as

$$\frac{dH_c}{dT_{D_2O}} = 0.34 \frac{\text{cm}}{^\circ\text{C}}$$

However, from the fitting process the uncertainty of ± 0.01 cm/°C could be evaluated.

The “experiment” of measurement of the dependence of the reactivity on the D<sub>2</sub>O temperature (*i. e.* the overall isothermal TCR) was based on a simple multiplication of the results of the measurements described in *Measurement of the reactivity gradient at the D<sub>2</sub>O critical level* for the value of the reactivity gradient  $d\rho/dH$  and obtained value for the  $dH_c/dT_{D_2O}$  shown above. The determined value for the overall isothermal TCR (taking in numerical round off) was reported in [12] as

$$\frac{d\rho}{dT} = (24 \pm 0.1) \cdot 10^{-4} \frac{1}{^\circ\text{C}}$$

The uncertainty of the D<sub>2</sub>O temperature measurements was not reported in published reports. Neither were given the data about calibration of the temperature measurements device (Platinum resistance thermometer connected in a Wheatstone bridge). The uncertainty of about 0.1 °C in the temperature values could be deduced from the graph presented in fig. 1 in [12] and from some temperature values given in the papers. It should also be noted that the reported value of the TCR was given in [12] without a related negative sign. The negative sign is evident, because the reactivity of the core decreases, *i. e.* the D<sub>2</sub>O critical level increases, with the rise of the temperature (fig. 1 in [12]).

### Measurements of the critical reactor geometrical parameter (buckling)

The experiment Measurement of the critical reactor geometrical parameter (buckling) is reported in [12]. The experiment was based on determination of the spatial distributions of the thermal neutron flux density along the central vertical axis of the core and along the diameter of the core at about half of the critical height of the D<sub>2</sub>O moderator. The spatial distributions of the thermal neutron flux density were determined by measuring activities of thin foils made of Dy and In, irradiated in the reactor core. Molar content of the moderator was reported as 99.76 % D<sub>2</sub>O. The corrections were applied due to the influence of the core surrounding materials, the increased D<sub>2</sub>O moderator critical height as a consequence of neutron absorptions in the foils and in the foil holders and the increased power of the reactor due to the irradiation process. The critical height of the D<sub>2</sub>O moderator during the irradiation was 182 cm [12]. To determine the thermal neutron flux density it was sufficient to measure the total activity of the In foils, without subtracting the epithermal neutron activity, [12]. Using the measured values of the  $dH_c/dT_{D_2O}$  (shown in *Measurement of the dependence of the D<sub>2</sub>O critical level on the temperature*), the measured geometrical parameters (buckling) were corrected to the D<sub>2</sub>O temperature of 20 °C. Using two-group diffusion theory, the buckling determination was done (1) under an assumption of the independence of the thermal neutron flux density spatial distributions in (vertical) axial and radial (horizontal) directions and (2) taking into account the values of the extrapolated dimensions in radial direction and axial directions (different extrapolated distances at the top and bottom of the core were determined). Several (15) measurements were done to determine the average thermal neutron flux density distribution in each (*r, z*) spatial direction.

Figure 2 in [12] shows a diagram of the average thermal neutron flux density (horizontal) distribution along the diameter of the core at (around) half of the critical height. Figure 3 in [12] shows a diagram of the average thermal neutron flux density (vertical) distribution along the central axis of the core. It can be seen that the irradiation positions of the foils in the core (used for the thermal neutron flux density spatial distributions), due to 15 independent measurements for each direction [12], were selected at average distance of 5 cm.

Fitting data for the average thermal neutron flux horizontal distribution from fig. 2 in [12] at Bessel function  $J_0(B_r r)$ , and applying the corrections mentioned above, the radial reactor geometrical parameter was determined as

$$B_r^2 = (5.576 \pm 0.016) \text{ m}^{-2}$$

Fitting data for the average thermal neutron flux vertical distribution from fig. 3 in [12] at sine function  $\sin(B_z z)$ , and applying the corrections mentioned above, the axial reactor geometrical parameter was determined as

$$B_z^2 = (2.940 \pm 0.012) \text{ m}^{-2}$$

The total reactor geometrical parameter (buckling,  $B_c^2$ ) was obtained by simply summing the reactor geometrical parameters (buckling) determined in the radial ( $B_r^2$ ) and axial ( $B_z^2$ ) directions, for the (extrapolated)  $H_c = (183.20 \pm 0.54) \text{ cm}$ , as

$$B_c^2 = B_r^2 + B_z^2 = (8.516 \pm 0.020) \text{ m}^{-2}$$

with a systematic "error" (uncertainty) estimated as "not higher than" 0.1 per m<sup>2</sup>.

The value of the total critical reactor geometrical parameter, was reported in [6], without any details on measurements, as

$$B_c^2 = (8.618 \pm 0.014) \text{ m}^{-2}$$

The buckling value, determined in the experiment mentioned above, correspond to the critical geometrical parameter of the RB system with the D<sub>2</sub>O critical level of 182 cm. Therefore, strictly speaking, this buckling value was not the geometrical parameter of the critical RB system with the D<sub>2</sub>O critical level of 177.60 cm, but was close to it.

### The migration length measurement

The migration length (*M*) measurement experiment was based on simple application of the modified one-group and two-group diffusion theory in which one can obtain (eq. 5 in [11]) relation between the migration area ( $M^2$ ), the critical height  $H_c$ , (determined in the section *Approach to the criticality*), the reactivity gradient  $d\rho/dH$  (determined in the section *Measure-*



ment of the reactivity gradient at the  $D_2O$  critical level), and the critical geometrical parameter  $B_c^2$  (the  $B^2$  determined in the section *Measurements of the critical reactor geometrical parameter (buckling)* assumed as equal to the critical one for the 177.60 cm  $D_2O$  moderator height) as

$$M^2 = \frac{\frac{d\rho}{dH}_c H_c^3}{2\pi^2 \cdot 0.5H_c^3 B_c^2 \frac{d\rho}{dH}_c}$$

By replacing the corresponding values obtained in the sections *Approach to the criticality*, *Measurement of the reactivity gradient at the  $D_2O$  critical level* and *Measurement of the critical reactor geometrical parameter (buckling)*, the squared value of the migration length ( $M^2$ , the “migration area”), for the  $H_c$  (extrapolated) = (183.20 ± 0.54) cm, was reported in [11] as

$$M^2 = (242 \pm 6) \text{ cm}^2 \text{ (two-group theory),}$$

or

$$M^2 = (270 \pm 6) \text{ cm}^2 \text{ (one-group theory)}$$

### Determination of the neutron multiplication factor in the infinite lattice

The experiment of determination of the “neutron infinite multiplication factor” ( $k_\infty$ ), i. e. neutron multiplication in the infinite lattice of the natural U metal fuel rods in the  $D_2O$  moderator with the square pitch of 12 cm was based on a simple application of two-group theory. In that theory, a relation (eq. 2 in [11]) between the neutron infinite multiplication factor  $k_\infty$ , the migration length  $M$  (determined in the section *The migration length measurement*) and the critical geometrical parameter  $B_c^2$  (determined in the section *Measurements of the critical reactor geometrical parameter (buckling)*), (under additional assumption that diffusion length ( $L$ ) is similar to Fermi age ( $\tau$ ) so that  $L^2 \approx \tau M^2/2$ ), for a critical system was obtained as

$$k_\infty = 1 + B_c^2 M^2 - 0.25 B_c^4 M^4$$

By replacing the corresponding values obtained in the section *Measurements of the critical reactor geometrical parameter (buckling)* and the section *The migration length measurement*, the value of the neutron infinite multiplication factor ( $k_\infty$ ) in the lattice natural U metal fuel rods in the  $D_2O$  moderator with the square pitch of 12 cm was reported in [11] as

$$k_\infty = 1.210 \pm 0.006$$

### Measurement of the safety rods reactivity

The experiment of Measurement of the safety rods reactivity is reported in [13]. Not all details about

the safety rods (SR) were given in the papers. Two safety rods were positioned at the reactor tank top cover, diametrically opposite and at 30 cm distance of the tank central vertical axis. The safety rods were made of stainless steel (SS) tube (3 cm in diameter, 170 cm long and with wall thickness of 2 mm). The SS tubes were lined inside by Cd sheet (1 mm thick) in the length of 50 cm extending from the lower end of the SS tube. No data were given about SS alloy or Cd material. The calculations of the SR reactivity (effective-ness) were done, assuming a pure black absorber with an effective radius, by the one-group theory and corrections were done by application of the two-group theory [13]. The perturbation theory was applied to account corrections due to the rod finite length and the rods non-central axis positions. The calculation results, using data from earlier experiments (the sections *Measurements of the critical reactor geometrical parameter (buckling)* and *The migration length measurement*) and assumed the total effective fraction of delayed neutrons and delayed photoneutrons of  $\beta = 0.0079$ , were also presented in [13] as  $\Delta k_1 = -0.0073$  (0.93 \$) for single SR and  $\Delta k_2 = -0.0137$  (1.74 \$) for both the SR. No uncertainty for the  $\beta$  value was given.

The experiment of measurement of reactivity of the SR was done by the “rod drop” technique, based on observation of time dependence of neutron flux density after sudden decrease of reactor reactivity (caused by the SR drop). In this experimental technique, if neutron flux density before drop of SR was recorded as  $n_0$  and  $n$  is observed neutron flux density when all delayed neutrons were died out, then the perturbation reactivity of the SR  $\delta k$  can be found from relation

$$n = n_0 \frac{\beta}{\beta - \delta k}$$

Correction were applied for the rod drop finite time and mathematical extrapolation done to find the correct ratio  $n_0/n$  in the experiment due to increased die out time of all delayed neutrons and delayed photoneutrons in a heavy water reactor [13].

Additionally, a variant of the rod drop experiment, referred as the Schultz method, based on the fact that the integral ratio of the neutron flux density, taken in some time interval before ( $n_0$ ) and immediately after the rod drop ( $n$ ), is proportional to  $\delta k/\beta$ , was applied too [13]. Details on the measurements, applying both rod drop techniques, were given in [13].

Both experimental methods were applied for each SR drop separately and for both SR drop together. A series of the SR drops were made and results of the SR reactivity, as a mean value within ± 5 % uncertainty, were reported in [13] as

#### The first rod drop method

Rod 1:  $\rho(\text{SR}_1) = 1.02$  \$; Rod 2:  $\rho(\text{SR}_2) = 1.00$  \$; Rods 1 + 2:  $\rho(\text{SR}_1 + \text{SR}_2) = 2.00$  \$.

\* Reactivity of 1 \$ =  $\beta$  value; (the non-SI unit \$ is often used as a reactivity unit in reactor kinetics or dynamics)

### *The second (Schultz) rod drop method*

Rod 1:  $\rho(\text{SR}_1) = 1.04 \$$ ; Rod 2:  $\rho(\text{SR}_2) = 1.04 \$$ ; Rods 1 + 2:  $\rho(\text{SR}_1 + \text{SR}_2) = 2.12 \$$ ,

with a note that the experiments have not shown the interference (*i. e.* the “shadowing effect”) of the reactivity between the two rods, what was predicted by the theoretical approach used. Again, the reported values of the reactivity of the safety rods in [13] were shown without the associated (obvious) negative sign, because the reactivity of the core was reduced by inserting the safety rods.

## CALCULATIONS

### Codes and libraries

This study is aimed to evaluate all the above mentioned RB reactor basic experiments and investigate their possibility for use in a validation of modern evaluated nuclear data files (ENDF). There had been large and productive experiences at the Vinča Institute in extensive and wide applications of many versions of the MCNP computer code (with different ACE type cross section libraries), at diverse models of complex reactor, transport and shielding systems (*e. g.* [20, 21]), since mid 1980es. The latest available production version (6.1) of the MCNP computer code [3] was selected for use in the ENDF validation at these RB basic reactor experiments (*Experiments*) made in 1958.

Only three recent ACE type libraries were chosen for this study:

- endf70 (extension: \*.70c), released by LANL in 2006 and based on the ENDF/B-VII.0 evaluated nuclear data files [22],
- endf71 (extension: \*.80c), released by LANL in 2011 and based on the ENDF/B-VII.1 evaluated nuclear data files [23], and
- jeff32 (extension: \*.03c), released by OECD/NEA in 2014 and based on JEFF-3.2 evaluated nuclear data files [24].

In this article, the small letters are adopted for names of the ACE formatted libraries and the capital letters were adopted for names of the evaluated nuclear data files. However, in the literature, the capital as well as small letters are used for names of both types of nuclear data libraries or files.

The LANL endf70 ACE type neutron only library is released for 390 isotopes and 3 elements and for 5 different temperatures (from 293.6 K to 2500 K) [25], out of which 293.6 K is the most appropriate for this study. The corresponding TSL ACE type neutron libraries are released for thermal neutron scattering at twenty moderators and for five to ten temperatures [26], from which one of 293.6 K is the only one appropriate for this study.

The LANL endf71 ACE type neutron only library is released for 423 nuclides and for 7 different tempera-

tures (from 0.1 K to 2500 K) [27], out of which 293.6 K is the most appropriate for this study. The corresponding TSL ACE type neutron libraries are released for thermal neutron scattering at ten moderators and for six to ten temperatures [28], out of which 293.6 K is the only one appropriate for this study.

The OECD/NEA jeff32 ACE type neutron only library is released for 473 nuclides and for 12 different temperatures (from 293.6 K to 1800 K) [24], out of which 293.6 K and 300 K are ones the most appropriate for this study. The corresponding TSL ACE type neutron libraries are released for thermal neutron scattering at nine moderators and for eight temperatures [24], among which 293.6 K is the only one appropriate for this study.

All evaluated nuclear data libraries, from the very early days, have kept growing in size, *e. g.* see [5], owing to adding (1) of data for more new isotopes (*i. e.* abandoning the elements' approach), (2) increasing precision of the evaluated and processed cross sections data, and (3) due to processing isotopes cross sections data at different temperatures. The new and extended TSL, *e. g.* see [5], with more precise evaluated cross sections data for thermal neutron scattering at more different moderator materials (molecules) and more temperatures, were also issued in that period.

In addition, from corresponding TSL, issued with the abovementioned three selected new libraries, the endf70Sab and jeff32Sab are of discrete type (for the energy of secondary neutron spectrum and angle distribution). The third TSL, the endf71Sab (first released officially with the MCNP6.1 [3]) uses new continuous type representation of these quantities. According to the report issued for the new endf71Sab TSL [28], these differences, in discrete and continuous representations of secondary neutrons data, should not influence the eigenvalue calculations, what this study should demonstrate as well.

Other (officially issued) recent evaluated nuclear data files (*e. g.* Japanese JENDL-4.0up3 or Russian BROND-3.2 and ROSFOND-2010) were not used in this study. These libraries were excluded from this study, because these libraries were not accompanied with the (own processed) ACE type libraries. Therefore, these libraries would require effort to any author to produce corresponding ACE type libraries by using the NJOY code [18], for use with the MCNP computer code for the RB1/1958 benchmark core. The NRG tendl2014 ACE type neutron library was also not used, because of the unsatisfactory evaluation results for isotopes bellow Fluorine, which was reported at the TENDL web site and confirmed (for the tendl2011) in the validations shown in [5].

### Data and models

In this validation study, all atom densities of the RB reactor materials were calculated for the material

composition isotopes. The exception was Zn, which neutron cross sections data in the endf70 were available only for the element material. The atom densities in the endf60 ACE library [16], used in [14], were given for the elements contained in the material composition. The exceptions were: the U metal (but not the impurities in the U), the B impurity, and the D<sub>2</sub>O moderator, for which the isotope atom densities were given. The Zn element ACE type cross sections, given in the vmccs library [17], used in [14] as well, were produced from the BROND 2 evaluated nuclear data file, using available version of the NJOY code [4] at the time.

All selected TSLs were used in this study at temperature of 293.6 K (20.45 °C), *i. e.* 25.301 meV, which was the closest to the reported experimental temperature (22 °C). The all other benchmark materials (natural U metal, SAV-1 cladding and tank material) were used also at 293.6 K. The exceptions were the D<sub>2</sub>O moderator and Air, which atomic densities were calculated at the experimental temperatures. For the Air inside the RB tank, above the D<sub>2</sub>O moderator critical level, it was assumed to have the same temperature as the D<sub>2</sub>O moderator and pressure which corresponds to the elevation of the RB reactor building at the Vinča Institute.

The benchmark model of the RB1/1958 core was chosen for use in this validation study of the experiments shown in the section *Experiments*. The selected benchmark model neglects all objects and equipment outside the RB tank top cover, the tank walls and the equivalent tank bottom. The reactor core was modelled with minimum approximations, which were evaluated too [14]. The safety rods (including the rods' guides) were not modelled, nor instruments (*e. g.* thermometer or the level measuring probes of the D<sub>2</sub>O moderator) inside the reactor tank. The influence of neutron reflection (back to the core) from the reactor room surfaces at the benchmark eigenvalue was evaluated as well [14]. The RB1/1958 model used in this study (the "study benchmark model", SBM) was the same as the benchmark model in [14], except that:

- the molar percent of the D<sub>2</sub>O content in the moderator was 99.79 % (as reported in [7]), instead of the evaluated value of 99.82 % shown in [14],
- the RB tank material was made of 99.9 (weight) % pure Al (as reported in [7]), with assumed 0.1 (weight) % of Si, instead of the assumed Yu\_Al material for the tank used in [14], and
- the Air pressure, which corresponds to the elevation (105 m above the sea level) of the RB building at the Vinča site, was taken at 22 °C, instead of the Air at sea level pressure and 20 °C, used in [14].

The content of 0.1 % (weight) impurities in the tank Al material was not reported in [7]. There is no certificate of the tank material composition in the RB reactor archive nowadays. Thus, the most common impurity element (Si) in high purity Al was chosen. The fact is that the RB tank is at the edge of the RB bare

core with a tiny influence at the eigenvalue of the criticality. An analysis, using the MCNP6.1 code and the endf71 library, has shown that the uncertainty in the RB tank material composition (either Yu\_Al, or SAV-1, or 100 % Al, or 99.9 % Al) influences the benchmark eigenvalue as  $17 \cdot 10^{-4}$ , *i. e.* far below the estimated uncertainty [14]. Similar sensitivity analysis has shown that change of 0.3 % (weight) in molar content of the H<sub>2</sub>O in the D<sub>2</sub>O moderator influences the eigenvalue of the benchmark model for  $(25.3 \pm 8.1) \cdot 10^{-4}$  [14], which is also within the uncertainty evaluated for this U-D<sub>2</sub>O core of the RB reactor. Therefore, these modifications, including the Air pressure-temperature, were considered a small change in the benchmark model. Other deviations from this SBM, if any, will be explained in the corresponding subsections of the section *Calculations*.

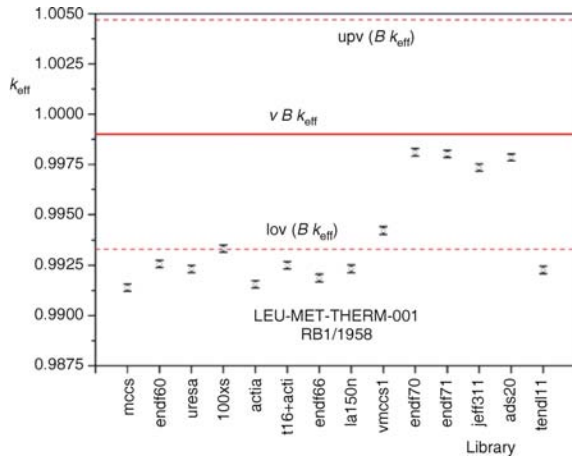
## Criticality

It was already mentioned that out of the RB reactor basic experiments performed in 1958 (and shown in the section *Experiments*), only the *Approach to the criticality* experiment was included as the evaluation LMT-001 (= LEU-MET-THERM-001 = RB-FUND-EXP-003) in the ICSBEP and IRPhEP Handbooks [14] in 1999. The experimental  $k_{\text{eff}}$  is 1.00000  $\pm$  0.00007, the evaluated benchmark  $k_{\text{eff}}$  is 0.9990  $\pm$  0.0057 in the LMT-001.

The version 4B2 of the MCNP computer code [15] with the endf60 [16] and the vmccs [17] ACE type neutron data libraries and neutron thermal scattering library (TSL) tmccs [18] were used in the LMT-001 evaluation in 1999. The code version and the neutron data libraries used are considered obsolete and have been superseded nowadays. Most of the available neutron data libraries (including TSL) of the ACE type (up to 2013) were used with newer version (5.1-6) of the MCNP computer code [19] in the validation process [5], which has also included the benchmark value of the RB assembly first core (RB1/1958) U-D<sub>2</sub>O moderator criticality data. These RB1/958 core validation results, given in Tables and Graphs in [5], were extracted from [5] and shown in this article as a graph in fig. 2. The older neutron data libraries, shown in fig. 2 at horizontal axis, are described (including TSL) briefly in [5].

The MCNP5-1.6 computer code was run for 10 million active neutron histories (10 Mnh) in all cases of the validations of the neutron nuclear data libraries [5]. These validation calculations with the MCNP5-1.6 code (in KCODE option) were done for 1 000 neutron active cycles, with 10 000 neutron histories in each cycle. The 100 neutron initial cycles were skipped. Such total number of the neutron histories ensured that MCNP5-1.6 code gave the neutron effective multiplication factor (eigenvalue,  $k_{\text{eff}}$ ), with an average uncertainty value (given as the statistical standard deviation  $1\sigma$ ) about  $(25 \pm 5) \cdot 10^{-5}$ . Only in cases of the vmccs and the endf60 libraries, the MCNP code results were taken





**Figure 2. Earlier [5] results of validation of the neutron data libraries for the RB1/1958 benchmark criticality experiment**

from earlier runs, done with smaller number of histories. Those results are not re-calculated, since they were given in the benchmark evaluation LMT-001.

The calculated data for  $k_{\text{eff}}$  are shown in the graph in fig. 2 with the symbols and associated the  $1\sigma$  uncertainties. Values of the benchmark  $k_{\text{eff}}$  eigenvalue ( $B k_{\text{eff}}$ ) are shown in the graph with solid line labelled with the " $v B k_{\text{eff}}$ ". The uncertainty limits in the value of the benchmark  $k_{\text{eff}}$  are shown in fig. 2 with dash lines labelled with as the " $upv (B k_{\text{eff}})$ ", *i. e.* the upper value of the ( $B k_{\text{eff}}$ ) and the " $lov (B k_{\text{eff}})$ ", *i. e.* the lower value of the ( $B k_{\text{eff}}$ ), respectively.

The endf71 ACE type library (with the endf71Sab TSL) shown in fig. 2 was issued by the NNDC (National Nuclear Data Center, Brookhaven National Laboratory, Uptown, USA), before the same labelled library was issued by the LANL (Los Alamos National Laboratory, Los Alamos, N. Mex., USA) with new version (6.1) of the MCNP code. A part of that ACE library (for temperatures above 300 K) was removed (later on in 2014) from the NNDC web site due to an error found in the NJOY-99.368 code, used for the processing data. The endf70 ACE type library (with the endf70Sab TSL), shown also in fig. 2, was released officially with the MCNP5-1.6 code, and was used in this study for the comparison. From fig. 2 it can be seen that older libraries (given at beginning of the fig. 2) and the tendl11 (from 2011) were not shown a satisfactory agreement with the benchmark eigenvalue value.

The effect of different, earlier available, TSL at the RB1/1958 benchmark eigenvalue was also examined and shown in [5]. Results obtained demonstrate that the effect of inclusion of various TSL at the  $k_{\text{eff}}$  was few hundreds pcm ( $1 \text{ pcm} = 1 \cdot 10^{-5} \Delta k/k$ ), except in the case of omitting the TSL, which was expected.

In this study, the MCNP.1 computer code was run for the SBM for 150 million active neutron histories (150 Mnh) in the KCODE mode. Initial 15 Mnh

were run firstly to obtain a fission neutron source equilibrium distribution in the SBM of the RB1/1958 core. Such number of 150 (active) Mnh ensured that the  $1\sigma$  uncertainty of the MCNP eigenvalue calculation was

0.00005, which was lower than reported experimental uncertainty (0.00007). The last uncertainty was estimated according to the reported uncertainty of the  $D_2O$  moderator critical height and the reported reactivity gradient at critical height. The  $D_2O$  moderator critical height of 177.60 cm [7] was assumed only in the SBM, *i. e.* the  $D_2O$  moderator critical height of 177.15 cm, reported in [6] was not used in this study. The calculation results for the values of the criticality were shown in tab. 1.

### Reactivity gradient at the $D_2O$ critical level

To determine calculated value of the reactivity gradient at the  $D_2O$  critical level, the MCNP6.1 computer code was run in the KCODE mode for active 25 Mnh, after initial 2.5 Mnh. Such number of active neutron histories ensured that the  $1\sigma$  uncertainty of the MCNP eigenvalue calculation was 0.00012, and the  $1\sigma$  uncertainty of the reactivity value was 0.00013. The increase of the heavy water over critical level ( $H$ ) was assumed +2.0 cm, which was corresponding to the experimental maximum overcritical value. The reactivity obtained in the calculations, as the relative change of the eigenvalues, was divided by the  $\Delta H$  value to obtain the reactivity gradient at the  $D_2O$  critical level, which was shown in tab. 1 and compared to the experimentally determined value.

### Dependence of the $D_2O$ critical level on the temperature

Value of dependence of the  $D_2O$  moderator critical level on the temperature was not possible to determine straightforward from the MCNP calculations, but it was determined from the formula shown below, after the (isothermal) temperature coefficient of reactivity (TCR) and the reactivity gradient (*Reactivity gradient at the  $D_2O$  critical level*) were calculated, according to the ratio

$$\frac{\frac{dH}{dT}}{\frac{d\rho}{dH}} = \frac{\frac{d\rho}{dT}}{\frac{d\rho}{dH}}$$

The reported experimental value of the (overall) isothermal TCR ( $-24 \text{ pcm/K}$ ) is given with the small ( $1\sigma$ ) uncertainty (1 pcm/K) in [12]. With the aim to calculate change of the reactivity with such a low uncertainty in the RB1/1958 core, with a small change of



**Table 1. Comparison of the results reported in the experiments and ones obtained by the MCNP6.1 code calculations**

Quantity	Experimental value ( <i>E</i> )	Calculation MCNP & ACE neutron data library value (C)								
		LANL endf71		(C – E)/E	LANL endf70		(C – E)/E	OECD/NEA jeff32		(C – E)/E
<i>k</i> <sub>eff</sub> at <i>H</i> <sub>c</sub> (cm), (exp: 1.00000 0.00007)	<i>H</i> <sub>c</sub> : 177.60 ± 0.10 <i>T</i> <sub>D2O</sub> : 22.0 °C %D <sub>2</sub> O: 99.79	0.99851	0.00005	–0.0015	0.99872	0.00005	–0.0013	0.99979	0.00005	0.0002
<i>dρ/dH</i> (10 <sup>–4</sup> cm <sup>–1</sup> )	7.06 0.15	7.86	0.65	0.11	5.56	0.65	–0.21	6.30	0.65	–0.11
<i>dH/dT</i> (cm/K)	0.34	0.10 ± 0.03		–0.71	0.19	0.05	–0.44	0.10	0.04	–0.71
<i>dρ/dT</i> <sup>(0)</sup> (10 <sup>–4</sup> K <sup>–1</sup> )	–2.4 0.1	–0.82	0.23	–0.64	–1.04	0.23	–0.57	–0.64	0.23	–0.73
<i>B</i> <sub><i>r</i></sub> <sup>2</sup> (m <sup>–2</sup> )	5.576 0.016	5.530	0.002	–0.01	5.527	0.001	–0.01	5.530	0.001	–0.01
<i>B</i> <sub><i>z</i></sub> <sup>2</sup> (m <sup>–2</sup> )	2.940 0.012	2.785	0.000	–0.05	2.764	0.000	–0.06	2.787	0.000	–0.05
<i>B</i> <sub><i>c</i></sub> <sup>2</sup> (m <sup>–2</sup> ) [7]	8.516 0.020	8.315	0.186	–0.02	8.291	0.140	–0.03	8.317	0.161	–0.02
<i>B</i> <sub><i>c</i></sub> <sup>2</sup> (m <sup>–2</sup> ) [6]	8.618 0.014			–0.04			–0.04			–0.03
<i>M</i> <sup>2</sup> (cm <sup>2</sup> ), <i>g</i> = 2	242 6	250.52	5.61	0.04	251.26	4.23	0.04	250.46	4.876	0.04
<i>M</i> <sup>2</sup> (cm <sup>2</sup> ), <i>g</i> = 1	270 6			–0.07			–0.07			–0.07
<i>k</i> <sub>∞</sub>	1.210 0.006	1.20831	0.00012 <sup>(1)</sup>	–0.0014	1.20834	0.00011 <sup>(1)</sup>	–0.0014	1.20869	0.00011 <sup>(1)</sup>	–0.0011
		1.20824	0.00011 <sup>(2)</sup>	–0.0015	1.20862	0.00011 <sup>(2)</sup>	–0.0011	1.20858	0.00011 <sup>(2)</sup>	–0.0012
		1.20817	0.00011 <sup>(3)</sup>	–0.0015	1.20814	0.00011 <sup>(3)</sup>	–0.0015	1.20862	0.00011 <sup>(3)</sup>	–0.0011
<i>β</i> (tot)	0.00790 <sup>(4)</sup> (assumed, [13])	0.00644	0.00017 <sup>(5)</sup>	–0.18	0.00699	0.00017 <sup>(5)</sup>	–0.12	0.00758	0.00015 <sup>(5)</sup>	–0.04
		0.00660	0.00018 <sup>(6)</sup>	–0.16	0.00677	0.00019 <sup>(6)</sup>	–0.14	0.00737	0.00020 <sup>(6)</sup>	–0.07
<i>ρ</i> <sub>SR1</sub> <sup>(0)</sup> (\$)	–1.02 <sup>(7)</sup> 0.05	–1.30	0.04 <sup>(5)</sup>	0.27	–1.20	0.03 <sup>(5)</sup>	0.18	–1.07	0.03 <sup>(5)</sup>	0.05
	–1.04 <sup>(8)</sup> 0.05			0.25			0.15			0.03
<i>ρ</i> <sub>SR2</sub> <sup>(0)</sup> (\$)	–1.00 <sup>(7)</sup> 0.05	–1.30	0.04 <sup>(5)</sup>	0.30	–1.20	0.03 <sup>(5)</sup>	0.20	–1.07	0.03 <sup>(5)</sup>	0.07
	–1.04 <sup>(8)</sup> 0.05			0.25			0.15			0.03
<i>ρ</i> <sub>SR1+SR2</sub> <sup>(0)</sup> (\$)	–2.00 <sup>(7)</sup> 0.10	–2.66	0.04 <sup>(5)</sup>	0.33	–2.48	0.03 <sup>(5)</sup>	0.24	–2.25	0.03 <sup>(5)</sup>	0.13
	–2.12 <sup>(8)</sup> 0.11			0.25			0.17			0.06

Notes: (0) experimental values of the TCR and  $\rho$ (SR) are shown in 2<sup>nd</sup> column with appropriate sign, (1) MCNP RB1 x-y cell Periodic boundary, (2) MCNP RB1 x-y cell Reflector boundary, (3) MCNP RB1 x-y cell White boundary, (4) no uncertainty was given for the assumed  $\beta$  value used by the experimentalists, (5)  $\beta$  value from MCNP prompt and total fission neutron eigenvalue calculations, (6)  $\beta$  value from MCNP6.1 mode KOPTS kinetics parameters, (7) rod drop, assumed 5 % uncertainty; (8) rod drop, Schultz method, assumed 5 % uncertainty

the D<sub>2</sub>O temperature ( $T = 5$  K) reported in the experiment, the MCNP6.1 computer code should run in the KCODE mode for a large number of neutron histories. A larger range of the  $T$  would allow shorter run of the MCNP6.1 code, but assumed linearity of the reactivity change with the temperature change in such wider temperature range would not be confirmed experimentally. It was estimated that the MCNP calculations (in parallel mode) would require around 250 Mnh. At one computer with a quad processor which has the speed of about 2.5 GHz, the 250 Mnh could be achieved in about 30 hours continuous run for only one case (*i. e.* one temperature value and one ACE type library). Such calculation would give the result of the reactivity (relative change of the eigenvalues obtained in two MCNP calculations) with 1 $\sigma$  uncertainty of 0.00005 (5 pcm).

Therefore, in order to avoid time consuming calculations, the value of the overall isothermal TCR was determined by the MCNP6.1 computer code for the critical level (177.60 cm) of the D<sub>2</sub>O moderator in two shorter runs for each ACE type library. One run was at the D<sub>2</sub>O moderator temperature of 20 °C and the other at 25 °C, which were the reported experimental mini-

mum and maximum moderator temperatures. Only atom densities of the D<sub>2</sub>O moderator and the Air were inserted in the MCNP input deck data at those two temperatures, while atom densities of all other materials in the core were given at the ACE library cross section temperature data (293.6 K). The jeff32 neutron library issued at 300 K, which is the closest to the experimental temperature of 25 °C, was not used for this calculation of the temperature dependence. The MCNP6.1 computer code was run for the SBM for only 50 million active neutron histories (after initial 5 Mnh) in the KCODE mode in each case. Such number of neutron histories ensured that the 1 $\sigma$  uncertainty of the MCNP reactivity calculation was 0.00011.

Therefore, such approach should give only rough values of the isothermal TCR with the proper (negative) sign with the 1 $\sigma$  uncertainty about 2.3 pcm/K for this validation study. The isothermal TCR could be obtained simply by division of the calculated reactivity by the temperature range (5 K), while a negative sign should show decrease of the reactivity with the temperature increase. The calculation results for the values of the isothermal TCR and the dependence of the D<sub>2</sub>O moderator critical level on the temperature were shown in tab. 1.

### Reactor critical parameter (buckling)

The calculated value of the critical reactor geometrical parameter for the RB1/1958 core was obtained by the least square fitting of the horizontal and vertical spatial distributions of the neutron flux density in the SBM obtained as the FMESH tally of the MCNP code for the thermal neutrons ( $E < 0.625$  eV) only. The height of the D<sub>2</sub>O moderator in the SBM was assumed equal to the experimentally reported (182 cm). The D<sub>2</sub>O moderator temperature of 22 °C was used in the calculations. The MCNP6.1 code was run for the active 25 Mnh, which ensured that the  $1\sigma$  statistical uncertainty of the FMESH tally values was below 0.4 % at any (of 23 chosen and equally spaced) bin of the FMESH tally. The vertical spatial distribution of the thermal neutron flux density was calculated along the vertical central axis ( $z$ ) of the reactor tank, from 0 cm to 230 cm. The horizontal spatial distribution of the thermal neutron flux density was calculated along the radius ( $r$ ) of the reactor tank, from the tank central axis ( $r=0$  cm) to the tank edge ( $r=105$  cm), at the approximately half ( $z=91$  cm) of the D<sub>2</sub>O moderator reported height. The experimental foils and their holders were not modelled due to missing data.

The radial (horizontal spatial) distribution of the thermal neutron flux density was fitted at the Bessel function of the first kind and integer zero order, *i. e.* to the  $AJ_0(B_r r)$ , from which the radial buckling  $B_r$  value was obtained. The axial (vertical spatial) distribution of the thermal neutron flux density was fitted at the sine function  $A \cdot \sin(B_z z + C)$ , from which the axial buckling  $B_z$  value was obtained. The calculated values of the thermal neutron flux density in points above the D<sub>2</sub>O critical level, for the vertical spatial distribution, were not used in the fitting process, because these points did not obey the sine function shape distribution. The fitting was done by using two independent numerical tools, the CURVEFIT code [29] and the ORIGIN software [30] in which was (additionally) implemented the required Bessel function, based on the polynomial approximation shown in [31]. Examples of the results of the fitting process for the FMESH tally calculated neutron flux density spatial distributions, using the jeff32 ACE type library, were shown in figs. 3 and 4. The obtained results for the geometrical buckling were given in tab. 1.

### Migration length

The migration length was calculated using the results of the MCNP6.1 code obtained for the neutron infinite multiplication factor and the critical geometrical parameter assuming the reactor was critical ( $k=1$ ). That critical condition of the reactor gave for a square of the migration length (*i. e.* the migration area), in the modified one-group, or two-group theory, a relation

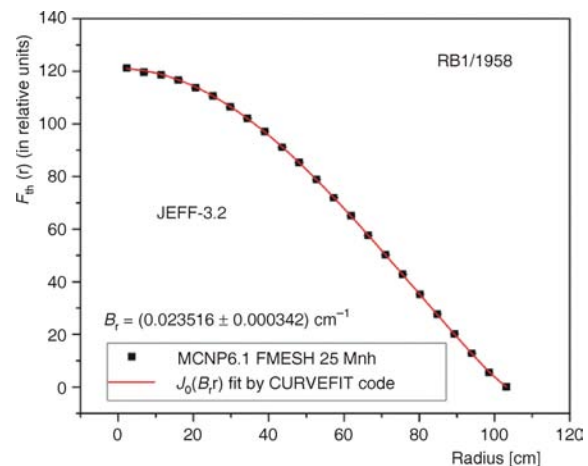


Figure 3. Calculated radial buckling  $B_r$  determination

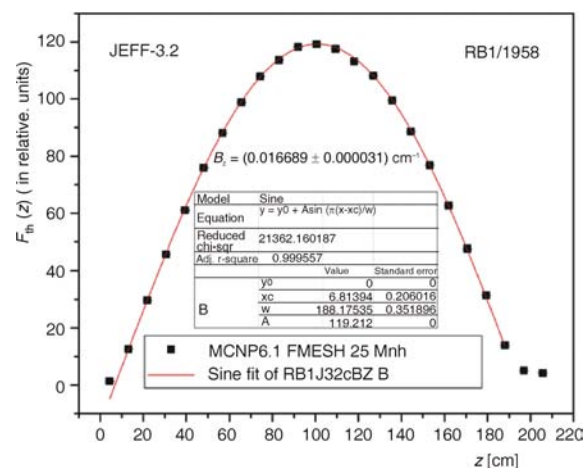


Figure 4. Calculated axial buckling  $B_z$  determination

$M^2 = (k_{\infty} - 1)/B_c^2$ . The calculated results were shown in tab. 1.

Another approach to calculate the migration area by the Monte Carlo method is based on a definition (*e. g.* [32, 33]), that the  $M^2$  is equal to 1/6 the average square of neutron track (crow-flight) path  $\langle r^2 \rangle$  in a (large) lattice. This Monte Carlo neutron “crow-flight” method assumes that each neutron history was followed along neutron tracks, from the spatial point (start) where neutron was born as the fast one (in fission) to the spatial point of its termination (absorption in a large reactor lattice with a negligible escape) as the thermal one. Using this intrinsic feature of the Monte Carlo methodology, the MCNP computer code may generate the PTRAC (particle track) file, from which the average square of the neutron crow-flight distance  $\langle r^2 \rangle$  may be extracted. The MCNP options, available to a user, allow selecting the SRC (neutron source) and the TER (neutron termination) events to record in the PTRAC file. The crow-flight distance of neutron is the minimal distance (*i. e.* the straight line) between the two (start, termination) spatial points mentioned, regardless the real

neutron path in a medium between these two points. The migration area was, then, simply calculated by division such obtained  $\langle r^2 \rangle$  value by six. The drawback of that method is that generated PTRAC file has a huge size, even in the case of demand for the minimum necessary information on neutron events recorded in it. For an example, the MCNP6.1 run for active 25 Mnh for the RB1/1958 core generates the PTRAC ASCII file of about 5 GB size. Additionally, the user has to write simple numerical code (*e. g.* FORTRAN) to extract the coordinates of the SRC and TER points, mentioned above, from the PTRAC file and calculate the  $\langle r^2 \rangle$  value.

Therefore, the MCNP6.1 code was run for 2.5 Mnh (neutron active tracks) for the RB1/1958 core SBM with all three ACE type neutron libraries and following values for the migration area were obtained by this method: (285.25 0.28) cm<sup>2</sup> (endf71); (284.06 0.24) cm<sup>2</sup> (endf70), and (283.34 0.24) cm<sup>2</sup> (jeff32).

It can be seen that these results for the  $M^2$  are from 6 % to 18 % higher than the experimentally reported ones. The obtained calculated value of the  $M^2$  for the endf70 ACE type library was also checked for 10-fold higher number of the neutron histories. The MCNP6.1 code was run, with the endf70 ACE type library, for 25 Mnh and the PTRAC ASCII file was generated with neutron (source and termination) events recorded in it. The obtained value of the  $M^2$  for the endf70 ACE type library was (262.77 0.07) cm<sup>2</sup>. This  $M^2$  value is between two reported experimental  $M^2$  values and is about 8 % less than the calculated one in the case of 2.5 Mnh, *i. e.* the neutron statistics issues have to be taken into account for this method. This method has also to include in data evaluation the fact that the RB1/1958 core was a large reactor lattice, but not with a negligible neutron escape from the core. The results of the MCNP6.1 calculations show that the neutron escape from the RB1/1958 core is 20 %. In particular, many of the natural U metal fuel rods were placed in the core near to the surface of the RB reactor tank wall in order to achieve a cylindrical, bare lattice with 12.0 cm square pitch. The probability of neutron escape from the RB reactor core for such fuel elements is higher than for ones placed around the centre of the core.

### Neutron infinitive multiplication factor

The neutron multiplication factor ( $k_\infty$ ) in the infinitive lattice of the natural uranium metal rod and the D<sub>2</sub>O moderator with square pitch of 12.0 cm was simply calculated by the MCNP6.1 code. A single square lattice cell of the SBM (12 cm pitch) with infinite dimension in axial direction, was selected and the MCNP6.1 code was run assuming the vertical surfaces of the cell with (1) periodic, (2) reflective, and (3) white boundary conditions for transport of neutrons. Spatial homogeneous fission neutron source, de-

scribed by the Watt neutron energy shape spectrum, was assumed in the fuel rod. The MCNP6.1 code was run for the active 25 Mnh, which enabled that the  $1\sigma$  statistical uncertainty of the eigenvalue (assumed to be equal to the  $k_\infty$ ) was 0.00012. The calculated results were shown in tab. 1.

### Reactivity of the safety rods

In order to calculate reactivity of the RB1/1958 safety rods, additional modifications and assumptions in the SBM were made. The SBM was modified by addition of the simplified model of two identical safety rods (SR). The assumptions in modelling the SRs were arisen due to the unknown details related to their (1) exact upper and lower positions in the reactor tank; (2) material compositions and (3) unknown rods' exact geometry.

The SR guide tubes and their moving mechanisms above the tank cover were not modelled. A part of the rods above the tank cover was neglected when the rods were in the upper positions. The wire, made of stainless steel, which holds the SR and was used for the rod moving, was also neglected. It was assumed that the SR outer diameter match exactly the rod penetrating hole in the top cover, when the rod was in the upper position (withdrawn), and that penetrating hole was completely closed by the top cover material when the rod was in the lower position (inserted).

The SR were modelled, according to the information given in [13], like the stainless steel (SS) tube with OD 3.0 cm, 170 cm long and 2 mm wide wall. Two SR were positioned diametrically opposite and at 30 cm distance of the tank central vertical axis. The inner bottom part of each safety rod SS tube was lined by Cd sheet, 1 mm thick and 50 cm long. No information was given about the position of the lowest end of the rod, when it was immersed in the reactor core. Based on the safety rods moving mechanisms, still in use at the RB reactor nowadays, it was assumed that the rod's bottom end has stopped at 50 cm above the tank bottom, when the SR was completely inserted in the core (the down position). Assuming that all RB tank geometry details, shown in fig. 2 in [7], were in scale, it was evaluated that the position of the bottom end of the SR in the upper position (withdrawn) was about 5 cm below the tank top grid plate, *i. e.* at 205 cm above the tank bottom. The uncertainty of these (upper, lower) ending positions of the SR was estimated at 5 cm. The rods' bottom conical ending (assumed made of SS), shown in the fig. 2 in [7], was not modelled. Inner space of the rod was filled by the Air with the pressure and the temperature same as the ones used for the Air in the RB tank above the D<sub>2</sub>O moderator critical level.

Information on exact material composition of the safety rod stainless steel tube was not given. Therefore, the SS type ANSI-430 (DIN X6Cr17) with mass



density of  $7.70 \text{ g cm}^{-3}$ , found at the RB storage, was assumed and modelled. The elemental (weight %) composition of this SS type is similar to the other SS types with Cr in range of (17–1) % and Fe in range of (60–5) %, with much smaller weight percent of impurities of other elements. No information was given on impurities in the Cd sheet material either, and, thus, 100 % pure Cd material was assumed with a theoretical mass density ( $8.65 \text{ g cm}^{-3}$ ). The effect of the uncertainties in composition of materials and geometrical dimensions at the SR reactivity was not evaluated, because it was out of the scope of this study.

The calculations of the SRs reactivity were carried out by running the MCNP6.1 computer code in the KCODE mode, for 25 Mnh, in three steps. In the first step, the eigenvalue ( $k_0$ ) of the modified SBM, with both safety rods completely withdrawn, was determined. In the second step, the eigenvalue ( $k_1$ ) of the modified SBM, with one safety rod (*e. g.* SR1) completely withdrawn and other safety rod (SR2) completely inserted, was determined. Since both safety rods were modelled identically, this step was used to determine the reactivity of either SR1 or SR2. The reactivity was determined as a relative change in the calculated eigenvalues:  $\rho = (k_1 - k_0)/k_0$ . In the third step, the eigenvalue ( $k_{12}$ ) of the modified SBM, with both safety rods completely inserted, was determined, and the reactivity of both safety rods was determined as  $\rho = (k_{12} - k_0)/k_0$ .

In order to compare the calculated reactivity of the SR with the reported experimental values, the calculated reactivity had to be shown in units of dollar (\$), *i. e.* divided by the total effective fraction ( $\beta$ ) of delayed neutrons and delayed photoneutrons. Therefore, the MCNP6.1 computer code was used to determine the value of the  $\beta$ , by two methods. In the first method, the MCNP6.1 computer code was run twice, in KCODE mode for 25 Mnh, to obtain the eigenvalue for (1) all neutrons from fission (total  $\nu$ ) and for (2) only prompt neutrons from fission (prompt  $\nu_p$ ). The value of the  $\beta$  was then obtained as relative change of such obtained eigenvalues. In the second method, the KOPTS option of the MCNP6.1 code was used, which gave straightforward the value of the  $\beta$  at the code output. Results of both calculations' options were shown in tab. 1, including the calculated reactivity of the safety rods given in dollars.

## RESULTS AND DISCUSSION

Results of the MCNP6.1 computer code calculations (C), with all three neutron ACE type libraries used are shown in tab. 1 and compared to the reported experimental (E) results. The comparison is shown in the columns labelled (C – E)/E associated to the columns with the calculated results for each ACE type neutron data library.

The calculated values of the neutron effective multiplication factor, at the reported D<sub>2</sub>O moderator critical height and the temperature of the RB1/1958 benchmark core, obtained for all examined ACE type neutron data libraries, are lower by only 0.15 % than the experimental eigenvalue. The best calculated eigenvalue value is achieved with the jeff32 ACE type neutron cross section data, that is only about  $(20–5) \cdot 10^{-5}$  less than the experimental eigenvalue. The endf70 and endf71 ACE type neutron cross section data libraries show the results which are  $130 \cdot 10^{-5}$  and  $150 \cdot 10^{-5}$  below the experimental value, respectively, which are also considered as very good agreements.

The calculated values of the reactivity gradient, at the reported D<sub>2</sub>O moderator critical height and the temperature of the RB1/1958 benchmark core, obtained for all examined ACE type neutron data libraries, are lower (between 11 % and 21 %) than the experimental value. The best calculated reactivity gradient value is again achieved with the jeff32 ACE type neutron cross section data.

The calculated overall isothermal TCR (*i. e.* dependence of the reactivity on the temperature) shows large discrepancy to the determined experimental value, higher than 50 %, for all used ACE type neutron data libraries. The trend (direction of change) of the reactivity with increase of the D<sub>2</sub>O moderator temperature is shown with proper negative sign for all libraries. In the case of the endf71 and jeff32 ACE type libraries the discrepancy to the experimental result is in the range of 65 % to 70 % for such small (5 K) temperature increase in the D<sub>2</sub>O moderator in the RB1/1958 core. Consequently, the change of the D<sub>2</sub>O moderator critical height with the temperature increase in such a small range (5 K) shows similar uncertainties. It is obvious that neutron cross sections data in all used ACE type libraries need further evaluation for such type of validation and the MCNP6.1 code should be run for much more neutron histories to achieve a better statistical uncertainty in the measured temperature range.

The calculated values of the radial geometrical reactor parameter (buckling), for all three used ACE type neutron libraries, are about 1 % less than the experimentally reported values, which is considered as a very good agreement. The calculated values of the axial geometrical reactor parameter (buckling), for all three used ACE type neutron libraries, are about 6 % less than the experimental reported values, which is considered as an expected result. Subsequently, the calculated values of the total geometrical buckling, for all three used ACE type neutron libraries, are different for about 4 % than the experimental reported value, which is considered a very good agreement.

The calculated values of the neutron infinite multiplication factor, for all used ACE type neutron cross section data libraries and all applied models of

the RB1/1958 reactor cell in the MCNP code, are only 0.1 % less than the experimentally determined value, which is a very good agreement.

The calculated values of the migration area, for all used ACE type neutron cross section data libraries, are only about 4 % less than the experimental value, reported for the (modified) two-group theory. These calculated values are only for about 7 % less than the experimental value, reported for the neutron modified one-group theory. The calculated values of the total geometrical parameter (buckling) and the calculated value of the neutron infinite multiplication factors were used in the same formula for determination of the migration length applied by the experimentalists. The comparison results are considered to be in good agreement.

In case of the “crow-flight” method, the MCNP calculated the migration area values were from 6 % to 18 % higher than the experimentally reported ones. It was shown that these discrepancies could be smaller if better statistic was used. The Monte Carlo method of calculation the migration area using determination of the average square of the neutron track path deserves more evaluation about its applicability, so obtained results were not included in tab. 1. That evaluation would include (if necessary) redefinition of the neutron path start event SRC (only fast neutron from fission) and the neutron path termination event TER (should be only thermal neutron absorption in the lattice, without escape), which are recorded in the PTRAC file. Such PTRAC file modification what would require editing of the MCNP6.1 code FORTRAN source file, inserting changes and recompiling the code, which option is not attainable to every one user of the MCNP code.

It can be seen that the calculated values of the effective neutron fraction of delayed neutrons and delayed photoneutrons,  $\beta$ , are smaller than the value  $\beta$  assumed by the experimentalists, in the range from 4 % to 16 %, depending on the method of the calculation used in the MCNP code and the used ACE type neutron data library. These discrepancies originate primarily from an incomplete contribution of delayed neutrons and delayed photoneutrons in the ACE type data libraries. In fact, neither used ACE type default neutron library shows delayed photoneutrons production in deuterium (of the D<sub>2</sub>O moderator, for gamma rays with energy higher than threshold, 2.225 MeV) or in other materials in the reactor core. However, it was possible, only in the case of the endf70 ACE type nuclear library, to combine default neutron library (\*.70c) with the photonuclear library (\*.70u) in order to account neutron production by photons. This was done in the MODE n p option of the MCNP6.1 code run for the same number of neutron histories. The KOPTS value  $\beta$  was not changed, but the value  $\beta$  obtained from two MCNP6.1 code runs gave higher value  $\beta$  (0.00735 0.00016), which was closer to the

value  $\beta$  assumed by the experimentalist, than one obtained for the endf70 library used without the photonuclear data library.

It is obvious that better agreements in the  $\beta$  value were obtained when the method of two (total and prompt neutrons from fission) runs of the MCNP6.1 code was applied than when the new KOPTS option in the MCNP6.1 code was used. Otherwise, the best agreement (about 4 %) of the calculated value of the  $\beta$  and the one assumed by the experimentalists was achieved for the jeff32 ACE type neutron data library and the method of two (total and prompt  $\nu$ ) runs of the MCNP6.1 computer code, since the jeff32 ACE type delayed photoneutron library is not available [24]. As the endf71 ACE type delayed photoneutron library is also not available in the default MCNP LANL distributed library collection, only the LANL la150 ACE type delayed photoneutron library can be still used, but with a limited number of nuclides.

The calculated reactivity of the safety rods in the RB1/1958 core shows discrepancy in range of 3 % to 33 %, depending of the ACE type neutron library. These differences are partially due to the simplified models of the safety rods. The calculated values of the  $\beta$  are used to express the calculated reactivity of the safety rods in dollars. However, if the experimentalists'  $\beta$  value would be used, the differences would be much smaller and would show more acceptable agreement. The best agreements were achieved when the results of the reactivity of the safety rods obtained in the calculations with the jeff32 ACE type neutron data library are compared to the reactivity of the safety rods determined experimentally by Schultz rod drop method.

## CONCLUSIONS

This study examined and evaluated measurements carried out at the natural uranium metal fuel lattices in the heavy water of the RB critical assembly first core, designed at the “Boris Kidrič” (now Vinča) Institute of Nuclear Sciences in 1958. The measurements performed at the RB reactor included seven basic reactor experiments to determine: the criticality; the reactivity gradient at the D<sub>2</sub>O critical level; the reactivity temperature coefficient; the critical reactor geometrical parameter (buckling); the migration length; the neutron infinite multiplication factor and the reactivity of the safety rods. With the aim to examine possible use of these experiments, as the benchmarks, for validation of modern nuclear data libraries, the results of the experiments are compared to the ones obtained using the MCNP6.1 computer code with three modern nuclear data libraries. A short overview of the experiments and used ACE type nuclear data libraries (endf71, endf70 and jeff32) is given. The RB1/1958 core benchmark model used for this validation study is briefly described and applied (with a

slight modification if necessary) to obtain requested computation results. The computations results are compared to the experimental ones in tab. 1. The acceptable agreements were found for all experiments, except for the isothermal temperature coefficient of reactivity (TCR) which requires further investigation of the obtained discrepancies. As the summary conclusion, among three ACE type neutron data libraries used in this validation study, the jeff32 data library showed the results closest to the experimental ones, except for the TCR. For possible inclusion of these experiments as the benchmarks in the IRPhEP, further evaluations of influences of missing data and uncertainties in material composition and geometry dimensions are required. Finally, it should be underlined that reactor experiments of these types and similar ones are still carried on at the various nuclear reactor facilities for basic research and education in the reactor physics worldwide nowadays, *e. g.* [34, 35].

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### **СТУДИЈА О КОРИШЋЕЊУ РЕАКТОРСКИХ ОСНОВНИХ ЕКСПЕРИМЕНАТА У U-D<sub>2</sub>O РЕШЕТКИ РЕАКТОРА РБ ЗА ВАЛИДАЦИЈУ САВРЕМЕНИХ БИБЛИОТЕКА НУКЛЕАРНИХ ПОДАТАКА**

Захтев за доступност добро дефинисаних реакторских експеримената за валидацију нумеричких програма у нуклеарној индустрији и технологијама је непрекидан. Корисници морају бити убеђени у резултате проверених нумеричких програма и библиотека нуклеарних података које су изабрали у моделима. Добро дефинисани (углавном „историјски”) и систематски евалуирани реакторски експерименти (њих око 5000 у 2015. години) сакупљају се непрекидно као стандарди (benchmarks) у оквиру OECD/NEA пројеката ICSBER (од 1995. године) и IRPhEP (од 2003. године) и објављују сваке године у електронском облику као међународни приручници.

Ова студија намењена је (а) испитивању и евалуацији реакторских основних експеримената, изведених у решетки природног уранијум метала и тешке воде у првом језгру на критичном реактору РБ (1958. године) и (б) приказу њихових могућности за валидацију савремених библиотека нуклеарних података. Ти основни реакторски експерименти укључују: (1) приближавање и одређивање критичности, (2) одређивање градијента реактивности на критичном нивоу тешке воде, (3) мерење зависности реактивности тешке воде од температуре, (4) мерење критичног геометријског реакторског параметра (buckling), (5) мерење миграционе дужине неутрона, (6) одређивање фактора умножавања неутрона у решетки бесконачних димензија, и (7) мерење реактивности сигурносних шипки. Резултати ових експеримената упоређени су са резултатима који су добијени коришћењем савремених нуклеарних података ACE типа кроз примену MCNP6.1, добро познатог и провереног нумеричког програма заснованог на методи Монте Карло. Дат је кратак приказ неутронских нуклеарних података ACE типа (креираних у LANL, заснованих на ENDF/B-VII.0 и ENDF/B-VII.1 датотекама евалуираних нуклеарних података, или у OECD/NEA, заснованих на JEFF-3.2 датотекама евалуираних нуклеарних података) коришћених у овој студији. Описан је бенчмарк модел коришћен у овој студији и добијени резултати су анализирани. Закључено је да су наведени основни реакторски експерименти у већини са природним уранијум металом у тешкој води реактора РБ, погодни за коришћење као стандарди за валидацију савремених библиотека нуклеарних података. То би се могло остварити након што се сви утицаји недостајућих података и неодређености у материјалном саставу и димензијама обраде према критеријумима и стандардима IRPhEP.

*Кључне речи: РБ реактор, U-D<sub>2</sub>O реакторски експеримент, MCNP6.1, библиотека нуклеарних података, валидација, IRPhEP*